AC 10801 ADVANCED SPECTROSCOPIC TECHNIQUES


Infrared Spectroscopy: Instrumentation and sample handling. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids, inorganic and organic compounds.


Electron Spin Resonance Spectroscopy - Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

References:
5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
AC 10802 NEWER METHODS IN ORGANIC SYNTHESIS


**Ionic Liquids:** Green Solvents, Reactions in acidic Ionic Liquids, Reactions in Neutral Ionic Liquids.

**References:**

1. Latest references (Reviews/Books) on the above topics.
AC 10803 ADVANCES IN ENVIRONMENTAL CHEMISTRY


Halo-organics and Pesticides: Chemistry of haloorganics: synthesis, reaction, microbial degradation and toxicity. Herbicides and organo-phosphorous insecticides: synthesis, reaction, environmental degradation and toxicity; Proposed phase out of all chlorine containing compounds.

Environmental Toxicology: Chemical solutions to environmental problems, biodegradability, Bioremediation of the environmental pollutants.

Emerging pollutants in the environment: Nanoparticles, pharmaceuticals: Chemistry, fate and transfer in the environment:

References:
2. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
7. Latest review articles/research papers
AC 10804 COMPUTATIONAL CHEMISTRY

Brief Idea about Quantum Mechanics:

Basic types of modeling techniques:

Basics of electronic structure theory:
Atomic units. The qualitative role of kinetic and potential energy in shaping the orbitals. Treating spin as an extra dimension.

Roothaan-Hall Hartree-Fock method.

Basis sets.
Basis set types: atomic, plane wave and grid basis sets. Atomic basis sets: Slater-type and Gaussian functions. Some frequently used basis sets: minimum, double and triple zeta basis sets, polarization and diffuse basis functions. Major semiempirical techniques.

Molecular properties and wavefunction analysis.
Orbital energies, Koopmans’ theorem, electrostatic properties. Canonical and localized molecular orbitals and their use in qualitative understanding of molecular properties. Symmetry (briefly).

Density Functional Theory (DFT).
Discussion of DFT techniques. History, advantages and critique. Major exchange-correlation functionals.

The calculation of equilibrium geometries, force constants, vibrational spectra, and transition states.
Gradient-based geometry optimization, the calculation of second derivatives, stability analysis. Reaction paths, the determination of transition states.

Electron correlation.
Comparison of configuration-based and density functional (DFT) techniques. MP2, CI and Coupled Cluster methods. Static and dynamic electron correlation.

Mathematical derivations excluded

TEXTBOOKS:
1. F. Jensen Introduction to Computational Chemistry
2. D C Young Computational Chemistry
3. C J Carmer Computational Chemistry
4. K. I. Ramachandran · G. Deepa ·and K. Namboori, Computational Chemistry and Molecular Modeling
Introduction
Definition, host-guest chemistry, supramolecular interactions, interdisciplinary nature of supramolecular chemistry

Host-Guest Chemistry or Molecular Recognition
Classification of host molecules/receptors: cation and anion binding hosts; cation-binding hosts (crown ethers, podands, cryptands, spherands, calixarenes, siderophores); nomenclature, solution behaviour, selectivity of cation complexation, macrocyclic, macrobicyclic and template effects, preorganization and complementarity, soft ligands for soft metal ions, complexation of organic cations, alkalides and electrides; anion-binding hosts

Crystal Engineering
Concepts, crystal structure prediction, the cambridge crystallographic structural database, crystal engineering of diamondoid lattices, crystal engineering with H-bonds, H-bonds to carbon monoxide, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides, π-π stacking, other interactions, awkward shapes and mismatch, coordination polymers, biomimetic structures, mixed crystals: hourglass inclusions

Self-Assembly
Introduction, biochemical self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, self-assembly of closed complexes by hydrogen bonding, catenanes and rotaxanes, halicates, molecular knots, catalytic and self-replicating systems

Molecular Devices
Introduction, supramolecular photochemistry, information and signals: semiochemistry, molecular electronic devices: switches, wires and rectifiers, machine based on catenanes and rotaxanes, dendrimers

Biological Mimics
Introduction, characteristics of enzymes, cyclodextrins as enzyme mimics, corands as ATPase mimics, cation-binding hosts as Transacylase mimics, metallobiosites, haem analogues, vitamin B_12 models

* The course will be offered as a pre-Ph.D course to the students who have not studied supra-molecular chemistry course at M.Sc.

Reference Books